



Full wwPDB EM Validation Report i

Nov 12, 2023 – 12:07 AM JST

PDB ID : 8W4J
EMDB ID : EMD-37266
Title : Cryo-EM structure of the KLHL22 E3 ligase bound to human glutamate dehydrogenase I
Authors : Su, M.-Y.; Su, M.-Y.
Deposited on : 2023-08-24
Resolution : 3.06 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) i) were used in the production of this report:

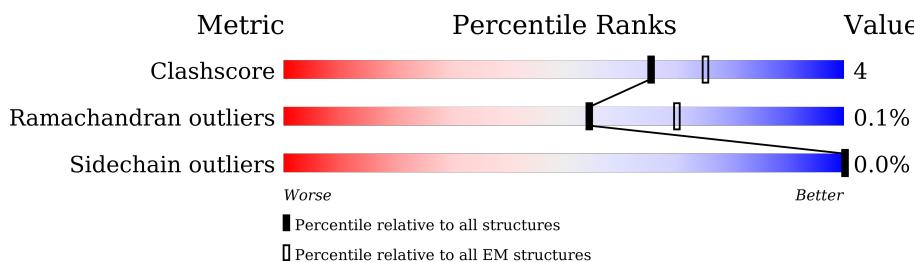
EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%



2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 27165 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	485	Total	C	N	O	S	0	0
			3510	2240	633	619	18		
1	B	484	Total	C	N	O	S	0	0
			3549	2266	639	627	17		
1	C	487	Total	C	N	O	S	0	0
			3600	2291	635	656	18		
1	D	486	Total	C	N	O	S	0	0
			3632	2303	642	670	17		
1	E	486	Total	C	N	O	S	0	0
			3611	2297	646	650	18		
1	F	487	Total	C	N	O	S	0	0
			3619	2301	646	654	18		

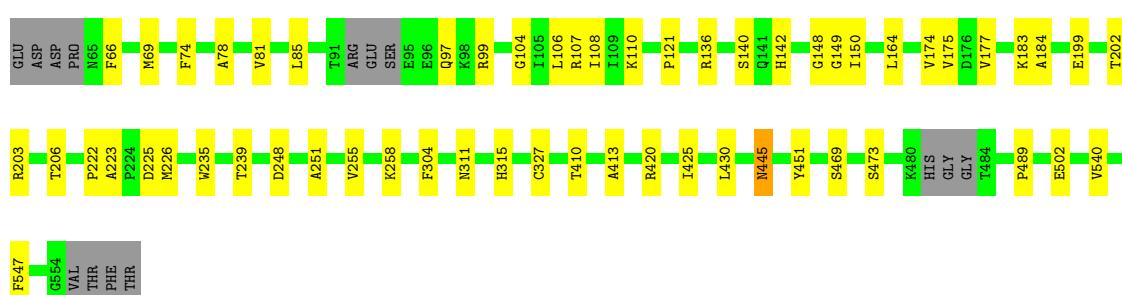
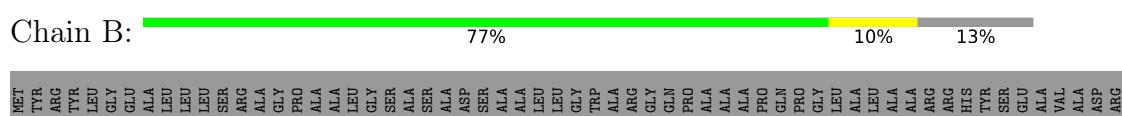
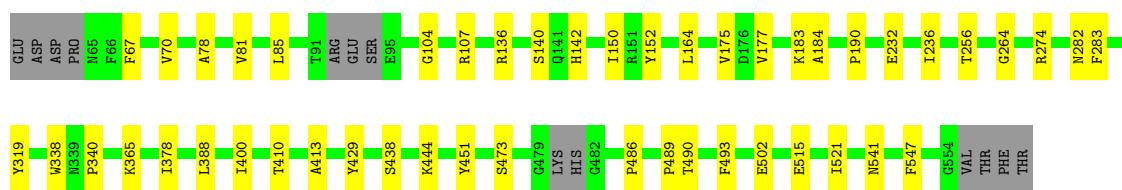
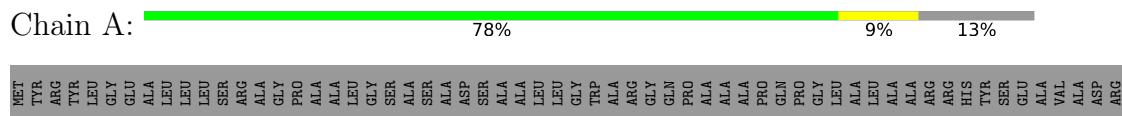
- Molecule 2 is a protein called Kelch-like protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	570	Total	C	N	O		0	0
			2812	1672	570	570			
2	J	574	Total	C	N	O		0	0
			2832	1684	574	574			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





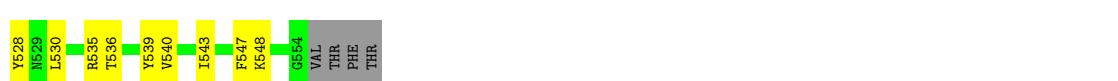
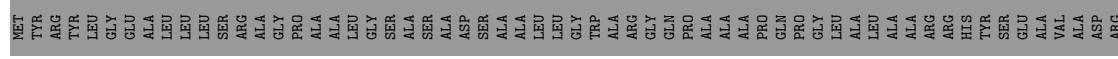
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain D: 76% 11% 13%



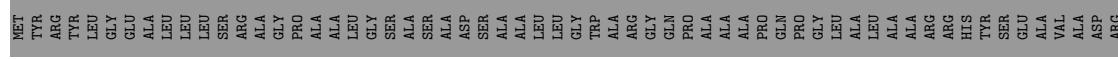
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain E: 75% 12% 13%



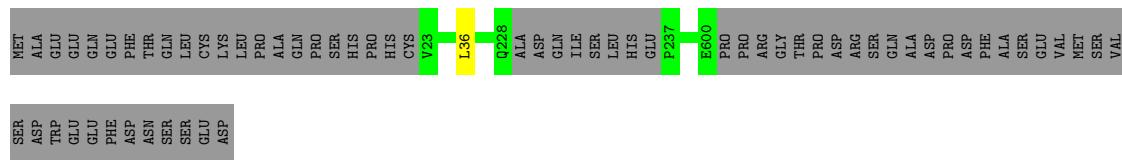
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F: 78% 9% 13%



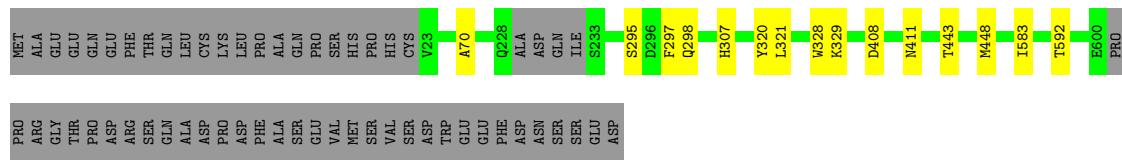
- Molecule 2: Kelch-like protein 22

Chain I:



- Molecule 2: Kelch-like protein 22

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62817	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.072	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	0/3587	0.47	0/4872
1	B	0.26	0/3627	0.48	0/4924
1	C	0.26	0/3679	0.48	0/4993
1	D	0.26	0/3710	0.47	0/5031
1	E	0.26	0/3690	0.48	0/5004
1	F	0.27	0/3698	0.48	0/5014
2	I	0.24	0/2810	0.44	0/3908
2	J	0.24	0/2830	0.44	0/3936
All	All	0.26	0/27631	0.47	0/37682

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	296	THR	Peptide

5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3510	0	3309	28	0
1	B	3549	0	3378	35	0
1	C	3600	0	3428	37	0
1	D	3632	0	3478	40	0
1	E	3611	0	3464	44	0
1	F	3619	0	3469	31	0
2	I	2812	0	1275	1	0
2	J	2832	0	1282	7	0
All	All	27165	0	23083	206	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TYR:HB2	1:B:502:GLU:HG3	1.73	0.70
1:A:378:ILE:HG22	1:A:400:ILE:HB	1.73	0.70
1:B:136:ARG:HD3	1:B:184:ALA:HB2	1.74	0.69
1:A:451:TYR:HB2	1:A:502:GLU:HG3	1.75	0.67
1:C:298:GLY:O	1:C:302:LYS:NZ	2.28	0.66
1:C:451:TYR:HB2	1:C:502:GLU:HG3	1.76	0.66
1:C:121:PRO:HB3	1:F:108:ILE:HD12	1.78	0.66
1:C:233:MET:HG2	1:C:236:ILE:HD12	1.79	0.65
1:A:264:GLY:O	1:A:444:LYS:NZ	2.31	0.64
1:C:468:MET:SD	1:C:471:GLN:NE2	2.69	0.63
1:C:459:GLU:O	1:C:463:ASN:ND2	2.30	0.63
1:F:338:TRP:HB2	1:F:367:TYR:HB2	1.81	0.63
2:J:321:LEU:HA	2:J:328:TRP:HA	1.82	0.62
1:C:191:LYS:O	1:C:191:LYS:HD2	1.99	0.61
1:E:222:PRO:HD2	1:E:255:VAL:HG12	1.82	0.61
1:C:462:SER:OG	1:E:496:ARG:NH2	2.33	0.61
1:C:193:TYR:HB3	1:C:197:GLU:HG3	1.82	0.61
1:A:283:PHE:HZ	1:A:521:ILE:HD11	1.66	0.60
1:C:204:ARG:NH1	1:C:208:GLU:OE2	2.34	0.59
1:C:489:PRO:HB3	1:C:493:PHE:HD2	1.67	0.59
1:F:337:ILE:HG23	1:F:364:ALA:HB1	1.85	0.59
1:D:230:GLU:OE1	1:D:268:ARG:NH2	2.36	0.59
1:D:490:THR:HG23	1:E:469:SER:HA	1.85	0.58
1:E:280:ILE:HD11	1:E:402:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:403:GLU:OE2	1:E:535:ARG:NH2	2.35	0.58
1:E:298:GLY:O	1:E:302:LYS:NZ	2.36	0.58
1:C:380:ILE:HG12	1:C:402:ALA:HB3	1.84	0.58
1:F:140:SER:HG	1:F:142:HIS:HD1	1.52	0.57
1:B:104:GLY:O	1:B:108:ILE:HG12	2.05	0.57
1:D:194:THR:OG1	1:D:197:GLU:OE1	2.15	0.57
1:D:147:LYS:NZ	1:D:256:THR:OG1	2.37	0.57
1:A:256:THR:HG21	1:A:438:SER:HB2	1.86	0.56
1:D:259:PRO:HG2	1:D:262:GLN:OE1	2.05	0.56
1:D:486:PRO:HA	1:E:473:SER:HB3	1.88	0.56
1:E:138:GLN:NE2	1:E:220:ASP:OD2	2.39	0.56
1:C:518:ALA:O	1:C:522:MET:HG2	2.05	0.55
1:C:425:ILE:HG21	1:C:430:LEU:HD13	1.87	0.55
1:D:136:ARG:HH11	1:D:184:ALA:HB2	1.73	0.54
1:B:121:PRO:HB3	1:D:108:ILE:HD12	1.90	0.54
1:C:209:LEU:HD23	1:C:215:ILE:HD13	1.90	0.53
1:F:142:HIS:HB3	1:F:550:TYR:CE1	2.43	0.53
1:D:451:TYR:HB2	1:D:502:GLU:HG3	1.91	0.53
1:E:136:ARG:HH11	1:E:184:ALA:HB2	1.74	0.53
1:D:104:GLY:O	1:D:108:ILE:HG12	2.08	0.53
1:D:222:PRO:HD2	1:D:255:VAL:HG22	1.91	0.53
1:B:410:THR:HG23	1:B:413:ALA:H	1.75	0.52
1:D:255:VAL:O	1:D:258:LYS:NZ	2.36	0.52
1:C:486:PRO:HA	1:D:473:SER:HB2	1.91	0.52
1:E:489:PRO:HB3	1:E:493:PHE:HD2	1.74	0.52
1:C:382:ALA:HA	1:C:405:ALA:HB2	1.92	0.52
1:A:164:LEU:HD23	1:A:183:LYS:HE2	1.92	0.52
1:D:315:HIS:CD2	1:D:318:ARG:HH21	2.28	0.51
1:F:104:GLY:O	1:F:108:ILE:HG12	2.10	0.51
2:I:36:LEU:HA	2:J:70:ALA:HB1	1.91	0.51
1:E:147:LYS:NZ	1:E:256:THR:OG1	2.44	0.51
1:A:152:TYR:HB3	1:A:190:PRO:HG3	1.91	0.50
1:D:281:GLU:HA	1:D:284:ILE:HG22	1.93	0.50
1:E:105:ILE:O	1:E:109:ILE:HG12	2.11	0.50
1:A:490:THR:HG23	1:A:493:PHE:H	1.75	0.50
1:C:140:SER:OG	1:C:142:HIS:ND1	2.41	0.50
1:E:144:THR:OG1	1:E:145:PRO:HD3	2.12	0.50
1:E:238:ASP:OD1	1:E:239:THR:N	2.45	0.50
1:D:489:PRO:HB3	1:D:493:PHE:HD2	1.76	0.50
1:F:142:HIS:HB3	1:F:550:TYR:HE1	1.74	0.50
1:E:410:THR:HG23	1:E:413:ALA:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG23	1:A:413:ALA:H	1.76	0.50
1:C:386:LYS:H	1:C:408:PRO:HA	1.77	0.50
1:F:471:GLN:HG3	1:F:486:PRO:HD2	1.92	0.50
1:D:140:SER:OG	1:D:142:HIS:ND1	2.35	0.49
1:B:222:PRO:HD2	1:B:255:VAL:HG12	1.94	0.49
1:D:104:GLY:O	1:D:107:ARG:HG2	2.12	0.49
1:E:528:TYR:CE2	1:E:540:VAL:HG11	2.48	0.49
1:C:230:GLU:HB2	1:C:259:PRO:HD3	1.94	0.49
1:C:467:LEU:HG	1:C:487:ILE:HA	1.95	0.49
1:A:282:ASN:ND2	1:A:515:GLU:HA	2.28	0.48
1:F:199:GLU:O	1:F:203:ARG:HG2	2.14	0.48
1:D:139:HIS:ND1	1:D:169:THR:HG21	2.28	0.48
2:J:408:ASP:N	2:J:411:ASN:O	2.45	0.48
1:F:153:SER:OG	1:F:155:ASP:OD1	2.24	0.48
1:A:338:TRP:O	1:A:365:LYS:N	2.45	0.48
1:A:104:GLY:HA2	1:A:107:ARG:HE	1.78	0.47
1:D:193:TYR:HB3	1:D:197:GLU:HB2	1.96	0.47
1:B:148:GLY:O	1:B:223:ALA:N	2.46	0.47
1:B:235:TRP:O	1:B:239:THR:HG22	2.14	0.47
1:F:394:PRO:O	1:F:420:ARG:NH1	2.47	0.47
1:C:530:LEU:HD13	1:C:536:THR:HG23	1.96	0.47
1:B:202:THR:O	1:B:206:THR:HG22	2.14	0.47
1:F:123:ARG:HE	1:F:127:GLY:HA2	1.79	0.47
1:B:108:ILE:HD12	1:D:121:PRO:HB3	1.96	0.47
1:E:82:GLU:O	1:E:86:VAL:HG23	2.14	0.47
1:B:425:ILE:HG21	1:B:430:LEU:HD13	1.95	0.47
1:D:337:ILE:HB	1:D:364:ALA:HB1	1.96	0.47
1:F:115:VAL:HG21	1:F:162:LYS:HD3	1.97	0.47
2:J:307:HIS:HA	2:J:583:ILE:HA	1.97	0.47
1:B:255:VAL:O	1:B:258:LYS:NZ	2.43	0.47
1:E:440:PHE:HD2	1:E:506:VAL:HG23	1.79	0.47
1:F:224:PRO:HA	1:F:233:MET:HE3	1.98	0.46
1:C:188:ILE:HD11	1:C:193:TYR:CZ	2.50	0.46
1:D:82:GLU:HG3	1:D:103:ARG:HD2	1.97	0.46
1:C:552:GLU:HB2	1:D:262:GLN:HE22	1.79	0.46
1:A:150:ILE:HD13	1:A:184:ALA:HB3	1.98	0.46
1:C:490:THR:HG23	1:D:469:SER:HA	1.98	0.46
1:F:276:VAL:HG12	1:F:430:LEU:HG	1.97	0.46
1:B:445:ASN:HD22	1:B:445:ASN:HA	1.62	0.46
1:B:164:LEU:HB3	1:B:183:LYS:HZ2	1.81	0.46
1:E:471:GLN:NE2	1:E:485:ILE:HG22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:320:TYR:O	2:J:329:LYS:N	2.49	0.46
1:C:307:GLN:O	1:C:383:ALA:HB2	2.16	0.45
1:E:485:ILE:O	1:E:485:ILE:HG13	2.16	0.45
1:C:488:VAL:HG21	1:D:476:ARG:HH12	1.81	0.45
1:E:402:ALA:HB1	1:E:430:LEU:HD21	1.97	0.45
1:D:199:GLU:O	1:D:203:ARG:HG2	2.15	0.45
1:F:142:HIS:CD2	1:F:143:ARG:HG2	2.51	0.45
1:C:539:TYR:O	1:C:543:ILE:HG12	2.16	0.45
1:D:309:PHE:O	1:D:352:LYS:NZ	2.49	0.45
1:B:174:VAL:HG13	1:B:175:VAL:HG13	1.98	0.45
1:D:484:THR:HG22	1:E:477:LYS:HE3	1.98	0.45
1:E:78:ALA:HB1	1:E:106:LEU:HD13	1.99	0.45
1:B:78:ALA:HB1	1:B:106:LEU:HD23	1.99	0.45
1:B:304:PHE:CZ	1:B:327:CYS:HB2	2.52	0.45
1:D:388:LEU:HB2	1:D:409:THR:HG22	1.99	0.45
1:A:274:ARG:NH2	1:A:319:TYR:OH	2.50	0.44
1:A:136:ARG:HH11	1:A:184:ALA:HB2	1.81	0.44
1:B:248:ASP:HB3	1:B:251:ALA:HB2	1.99	0.44
1:A:175:VAL:HG23	1:A:177:VAL:HG23	2.00	0.44
1:E:276:VAL:HG12	1:E:430:LEU:HG	2.00	0.44
1:A:338:TRP:CZ2	1:A:340:PRO:HG3	2.53	0.44
1:E:338:TRP:CZ2	1:E:340:PRO:HG3	2.52	0.44
1:E:85:LEU:O	1:E:103:ARG:NH2	2.50	0.44
1:A:85:LEU:HD21	1:A:547:PHE:CD2	2.53	0.44
1:A:140:SER:OG	1:A:142:HIS:ND1	2.32	0.44
2:J:443:THR:HA	2:J:448:MET:HA	2.00	0.44
1:A:232:GLU:O	1:A:236:ILE:HG13	2.18	0.43
1:F:264:GLY:O	1:F:444:LYS:NZ	2.37	0.43
1:F:136:ARG:HD2	1:F:184:ALA:HB2	1.99	0.43
1:E:420:ARG:HG3	1:E:422:ILE:HG12	2.00	0.43
1:B:199:GLU:O	1:B:203:ARG:HG2	2.19	0.43
1:F:311:ASN:OD1	1:F:315:HIS:ND1	2.51	0.43
1:B:107:ARG:NH1	1:D:129:TRP:O	2.51	0.43
1:B:150:ILE:HD13	1:B:184:ALA:HB3	2.01	0.43
1:C:136:ARG:HD3	1:C:184:ALA:HB2	1.99	0.43
1:D:332:GLU:HG2	1:D:333:SER:H	1.84	0.43
1:E:147:LYS:NZ	1:E:223:ALA:HB2	2.34	0.43
1:E:311:ASN:OD1	1:E:315:HIS:ND1	2.52	0.43
1:C:304:PHE:HB3	1:C:378:ILE:HB	2.00	0.43
1:F:90:ARG:NH1	1:F:551:ASN:OD1	2.52	0.43
1:F:122:ILE:HG21	1:F:201:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:LEU:HD12	1:D:430:LEU:HA	1.88	0.43
1:E:147:LYS:HD2	1:E:221:VAL:HG13	2.01	0.43
1:A:521:ILE:HG22	1:A:541:ASN:HD22	1.84	0.42
2:J:297:PHE:HA	2:J:592:THR:HA	2.00	0.42
1:B:74:PHE:CE2	1:B:110:LYS:HB2	2.54	0.42
1:B:140:SER:OG	1:B:142:HIS:ND1	2.39	0.42
1:E:338:TRP:O	1:E:364:ALA:HB1	2.20	0.42
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.85	0.42
1:F:429:TYR:OH	1:F:514:MET:O	2.38	0.42
1:F:429:TYR:OH	1:F:518:ALA:HB2	2.20	0.42
1:A:67:PHE:HA	1:A:70:VAL:HG12	2.01	0.42
1:A:283:PHE:HE2	1:A:429:TYR:CE2	2.38	0.42
1:B:66:PHE:HA	1:B:69:MET:HG2	2.02	0.42
1:B:81:VAL:CG2	1:B:540:VAL:HG23	2.50	0.42
1:B:420:ARG:HE	1:B:420:ARG:HB3	1.71	0.42
1:A:486:PRO:HA	1:B:473:SER:OG	2.20	0.42
1:E:403:GLU:HB3	1:E:427:ASP:HB3	2.02	0.42
1:F:85:LEU:HD21	1:F:547:PHE:CD2	2.54	0.42
1:A:473:SER:HB2	1:F:486:PRO:HA	2.02	0.41
1:B:225:ASP:OD1	1:B:226:MET:N	2.46	0.41
1:C:430:LEU:HD12	1:C:430:LEU:HA	1.90	0.41
1:C:136:ARG:HD2	1:C:183:LYS:O	2.20	0.41
1:E:530:LEU:HD13	1:E:536:THR:HG23	2.02	0.41
1:C:78:ALA:HA	1:C:81:VAL:HG12	2.02	0.41
1:D:150:ILE:HG12	1:D:184:ALA:HB3	2.02	0.41
1:D:416:ILE:O	1:D:420:ARG:HG2	2.21	0.41
1:D:471:GLN:HB2	1:D:486:PRO:HG2	2.03	0.41
1:E:145:PRO:HB2	1:E:179:PHE:CD1	2.56	0.41
1:A:489:PRO:HA	1:B:469:SER:HB3	2.01	0.41
1:C:78:ALA:HB1	1:C:106:LEU:HD13	2.02	0.41
1:F:257:GLY:N	1:F:441:GLU:OE1	2.44	0.41
1:B:175:VAL:HG23	1:B:177:VAL:HG23	2.01	0.41
1:B:311:ASN:OD1	1:B:315:HIS:ND1	2.52	0.41
1:B:489:PRO:HA	1:F:469:SER:HB2	2.03	0.41
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.92	0.41
1:E:539:TYR:O	1:E:543:ILE:HG12	2.20	0.41
1:E:116:LEU:HD21	1:E:118:LEU:HD21	2.03	0.41
1:C:394:PRO:HA	1:C:420:ARG:HH22	1.86	0.41
1:D:232:GLU:O	1:D:236:ILE:HG13	2.20	0.41
1:E:236:ILE:CD1	1:E:255:VAL:HG11	2.51	0.41
1:D:230:GLU:HB2	1:D:259:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:ASN:ND2	1:F:363:LYS:O	2.54	0.41
1:D:122:ILE:HG13	1:D:201:ILE:HD13	2.02	0.40
1:E:85:LEU:HD21	1:E:547:PHE:CD2	2.55	0.40
1:E:416:ILE:HD12	1:E:416:ILE:H	1.85	0.40
1:E:548:LYS:HE2	1:E:548:LYS:HB2	1.90	0.40
1:F:145:PRO:HB2	1:F:179:PHE:CD1	2.56	0.40
1:B:85:LEU:HD21	1:B:547:PHE:CE2	2.56	0.40
1:C:392:ASN:OD1	1:C:392:ASN:N	2.55	0.40
1:B:97:GLN:H	1:B:99:ARG:NH1	2.19	0.40
1:B:149:GLY:HA2	1:B:223:ALA:O	2.21	0.40
1:D:510:LEU:O	1:D:514:MET:HG2	2.21	0.40
1:E:296:THR:O	1:E:302:LYS:NZ	2.45	0.40
1:F:403:GLU:OE2	1:F:535:ARG:NH2	2.48	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.97	0.40
1:E:159:ASP:N	1:E:159:ASP:OD1	2.53	0.40
1:E:474:LEU:HD23	1:E:474:LEU:HA	1.86	0.40
1:F:290:MET:HB3	1:F:296:THR:HA	2.04	0.40
1:A:78:ALA:HA	1:A:81:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	479/558 (86%)	457 (95%)	22 (5%)	0	100 100
1	B	478/558 (86%)	457 (96%)	21 (4%)	0	100 100
1	C	481/558 (86%)	458 (95%)	23 (5%)	0	100 100
1	D	480/558 (86%)	456 (95%)	24 (5%)	0	100 100
1	E	480/558 (86%)	462 (96%)	18 (4%)	0	100 100
1	F	483/558 (87%)	449 (93%)	32 (7%)	2 (0%)	34 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	566/634 (89%)	554 (98%)	12 (2%)	0	100 100
2	J	570/634 (90%)	556 (98%)	12 (2%)	2 (0%)	34 64
All	All	4017/4616 (87%)	3849 (96%)	164 (4%)	4 (0%)	54 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	296	THR
1	F	297	PRO
2	J	295	SER
2	J	298	GLN

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/452 (72%)	324 (100%)	0	100 100
1	B	335/452 (74%)	334 (100%)	1 (0%)	92 96
1	C	350/452 (77%)	350 (100%)	0	100 100
1	D	360/452 (80%)	360 (100%)	0	100 100
1	E	352/452 (78%)	352 (100%)	0	100 100
1	F	353/452 (78%)	353 (100%)	0	100 100
All	All	2074/2712 (76%)	2073 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	445	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.